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Boundary elements in steady convective diffusion problems

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Abstract: A boundary element method is developed to solve the steady convective diffusion equation in n dimensions. For the formation a transformation into the selfadjoint or symmetric operator is used under a certain assumption, and a boundary integral equation is derived from the Green's second identity. For the discretization of the boundary integral equation, constant or linear boundary elements are employed. A simple model problem is treated in numerical experiments, and a comparison with the finite element methods is given. It is shown that the present boundary element solution is stable with respect to large Peclet numbers and is with the second-order accuracy.

Keywords: Integral equation, boundary elements, convective diffusion equation.

1. Introduction

Convective diffusion equation is known as the governing equation on heat or mass transfer phenomena [14]. The equation has been, to the present, solved by some domain-type methods such as the finite difference method [14] and the finite element method [5,20]. Most of them however give rise to oscillatory and nonphysical solutions for large Peclet numbers [5,10,14,20]. In order to suppress such the oscillatory solutions the upwind methods [4,14], the method of adaptive mesh refinement [3] and the other methods [10] have been developed. In particular the upwind or Petrov–Galerkin finite element method [3,4,12] has had a wide use for practical applications. But the upwind method is not always effective in the attainable accuracy and the saving of computational cost.

On the other hand, the boundary element method [1,2], one of the boundary-type methods, has been applied to many practical problems in engineering [2], and its usefulness has been recognized gradually.

In the most recent years, some boundary element methods have been developed to solve the steady and transient convective diffusion equations. Ikeuchi, Sakakihara and Onishi [7] have first presented the boundary element solution for the steady convective diffusion equation with plugged or uniform flow in three dimension by means of the direct formulation [1]. Ikeuchi and Onishi [6], and Skerget and Brebbia [18] have dealt with the plane-Poiseille flow by regarding the convective term as a body force added to the pure diffusion equation. In addition, Matsunashi [11] has dealt with more general potential flow. The boundary element solutions presented [7,8,18] have been stable with respect to large Peclet numbers.

In the paper a boundary element method for the steady convective diffusion equation in n dimensions is presented that differs from the previously published ones. The formulation is based

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on a transformation of the convective diffusion operator into the selfadjoint or symmetric operator and on an application of the Green's second identity. The resulting boundary integral equation is discretized by use of the constant or linear boundary elements. Through a simple example it will be shown that the boundary element solution is stable with respect to large Peclet numbers and is superior in the accuracy to the standard and upwind finite element solutions.

2. Convective diffusion equation

Let Ω be a bounded open domain in $\mathbb{R}^n$ enclosed by the smooth boundary Γ. Assume that Ω is occupied with homogeneous and isotropic medium, and that ϕ is the temperature (or scalar function) under consideration. The time-independent heat transfer problem is then expressed by the steady convective diffusion equation

$$-\nabla\cdot(\alpha\nabla\phi)+c\rho(v\cdot\nabla)\phi=p \quad \text{in} \quad \Omega \tag{1}$$

where α is the thermal conductivity, c is the specific heat, ρ is the density, v is the velocity vector, and p is the heat source.

Equation (1) becomes nonlinear if α depends on ϕ. For this nonlinear case we can prepare the Kirchoff's transformation defined by

$$\Phi=\int_{\phi_0}^{\phi}\alpha(\phi)\,\mathrm{d}\phi \tag{2}$$

where ϕ_0 is an arbitrary reference value [17]. The application of (2) to (1) gives

$$-\nabla^2\Phi+2(V\cdot\nabla)\Phi=p \quad \text{in} \quad \Omega \tag{3}$$

where $V=v/(2\kappa)$ for the diffusivity $\kappa=\alpha/(c\rho)$ of which the magnitude means the Peclet number (Pe). Here κ can be approximated by a constant diffusivity because it does not so strongly depend on Φ in practical applications. If α depends only on the space variable $x=(x_i)$ then we may be possible to use a transformation of the variable

$$\xi=\int_{x_0}^{x}(1/\alpha)\,\mathrm{d}x \tag{4}$$

for (1), in which x_0 is an arbitrary reference point. With respect to the new variable ξ, (1) can be reduced to the same form with (3). Of course, if α is the constant conductivity then (1) can be directly rewritten into (3).

Therefore we shall study on the solution to (3) in what follows. In addition to (3) we must impose the boundary conditions

$$\Phi=\overline{\Phi} \qquad \text{on} \quad \Gamma^{(1)} \tag{5a}$$

and

$$Q=\partial\Phi/\partial n=\overline{Q} \quad \text{on} \quad \Gamma^{(2)} \tag{5b}$$

where $\overline{\Phi}$ and $\overline{Q}$ are respectively the prescribed values on $\Gamma^{(1)}$ and $\Gamma^{(2)}$, in which $\Gamma=\Gamma^{(1)}+\Gamma^{(2)}$ and n denotes the outer normal to Γ.

3. Boundary integral equation

The convective diffusion equation (3) under consideration becomes non-selfadjoint for the dominant convection. This fact leads to oscillatory solutions in the conventional application of the domain-type methods to (3). Thus we attempt to transform (3) into a selfadjoint or symmetric expression.

At first we prepare the transformation formula defined by

$$\Phi = \exp(F)u \tag{6}$$

where we must make the following assumption: there exists a scalar flow potential $F(x)$ such that

$$V = \nabla F \tag{7}$$

for all $n(\geqslant 1)$. Rigorously speaking, this assumption is not always valid excepting $n = 1$. The application of (6) to (3) yields

$$L[u] = -\nabla^2 u + \left(|\nabla F|^2 - \nabla^2 F\right)u = b \quad \text{in} \quad \Omega \tag{8}$$

where $b(x)$ given by

$$b = \exp(-F)p. \tag{9}$$

Notice that Tabata [19] has recently formulated a finite element scheme for (8). Before we proceed to the boundary integral equation formulation, we rewrite by use of (6) the boundary conditions (5a) and (5b) as follows:

$$u = \exp(-F)\overline{\Phi} = \bar{u} \qquad \text{on} \quad \Gamma^{(1)} \tag{10a}$$

and

$$q + V_n u = \exp(-F)\overline{Q} = \bar{h} \quad \text{on} \quad \Gamma^{(2)} \tag{10b}$$

in which $q = \partial u/\partial n$, and $V_n(=\partial F/\partial n)$ is the n component of V. Here the pure Neumann condition (5b) has been transformed into the Robin condition (10b) in which V_n must satisfy the Hölder condition [2].

Since L is selfadjoint, the Green's second identity can be simply expressed as

$$\int_\Omega \{wL[u] - uL[w]\}\,\mathrm{d}\Omega = \int_\Gamma \{u(\partial w/\partial n) - w(\partial u/\partial n)\}\,\mathrm{d}\Gamma \tag{11}$$

where w is an adjoint potential field to u. Suppose that we know a fundamental (or elementary) solution $w^*(P_i, P)$ satisfying

$$L[w^*] = \delta(P_i, P) \quad \text{in} \quad \mathbb{R}^n \tag{12}$$

in which $\delta(\cdot)$ denotes the Dirac's delta function at an arbitrary point P_i, and P is the reference point. Taking w^* instead of w in (11) and substituting (8) into (11), we obtain the boundary integral equation

$$a(P_i)u(P_i) + \int_\Gamma q^*(P_i, P)u(P)\,\mathrm{d}\Gamma = \int_\Gamma w^*(P_i, P)q(P)\,\mathrm{d}\Gamma + \int_\Omega w^*(P_i, P)b(P)\,\mathrm{d}\Omega \tag{13}$$

where $a(P_i)$ is some weight depending on the solid angle of Ω at the point P_i, and $q^* = \partial w^*/\partial n$. Here the left-hand side integral in (13) should be interpreted in the Cauchy's principal value sense. Note that the derivation of $a(P_i)$ will be given later.

4. Fundamental solution

Let us consider the fundamental solution w^* for the specified flow potential F by

$$-\nabla^2 F + |\nabla F|^2 = C \quad \text{in} \quad \Omega \tag{14}$$

in which C is assumed to be a real constant. Equation (12) can be then expressed as

$$L[w^*] = -\nabla^2 w^* + Cw^* = \delta(P_i, P) \quad \text{in} \quad \mathbb{R}^n \tag{15}$$

where for $C > 0$, $= 0$ and < 0 L is classified into the modified Helmholtz (or steady Klein–Gordon) operator, the Laplacian and the Helmholtz operator, respectively. Therefore we can easily know w^* in (15) for any C. At the same time we must solve (14) since F is required for (6). Equation (14) is the Ricatti-type equation which cannot be always solved analytically excepting $n = 1$, but if there exists the scalar function U such that $\nabla F = -\nabla U/U$ then (14) may be reduced to $L[U] = 0$. Thus under the assumption of $\nabla^2 F (= \nabla \cdot V) \neq 0$, we can derive both w^* and F (or V) for some special cases [9] from (14) and (15).

For simplicity we impose $\nabla^2 F = 0$ on (14) and (15) which means the incompressible flow in Ω. The case of $C = 0$ readily attains to $V = 0$, and the case of $C < 0$ becomes illogical. Thus we consider only the case of $C = \mu^2 > 0$, i.e., the uniform velocity field. By use of the Fourier and its inverse transformations for (15) [9,13] we obtain $w^* = w_n^*$ for $n = 1$, as

$$w_1^* = \exp(-\mu R)/(2\mu) \tag{16}$$

where the subscript n denotes the dimension in spaces, $\mu > 0$ and R is the distance between P_i and P. Since w_n^* depends only on R, we can employ the formulas [13]

$$w_2^* = \int_{-\infty}^{+\infty} w_3^*(R)\, \mathrm{d}x_3 \tag{17a}$$

and

$$w_3^* = -(1/2\pi R)\left[\mathrm{d}w_1^*(x_1)/\mathrm{d}x_1\right]_{x_1 = R}. \tag{17b}$$

In the result we know

$$w_2^* = K_0(\mu R)/(2\pi) \tag{18}$$

and

$$w_3^* = \exp(-\mu R)/(4\pi R) \tag{19}$$

where $K_0(\cdot)$ denotes the modified Bessel's function of the second kind of order zero.

For such the fundamental solution w^* presented above, the left-hand side integral in (13) contains a strong singularity at $P_i = P (\in \Gamma)$ which is integrable only in a concept of the Cauchy's principal value. Therefore we must take into account the following limiting process (see Fig. 1): for example, in the case of $n = 2$

$$(1/2\pi) \lim_{\varepsilon \to 0} \int_{\Gamma_\varepsilon} [\partial K_0(\mu\varepsilon)/\partial n]\, u(P)\, \mathrm{d}\Gamma = [(\theta_1 - \theta_2)/2\pi]\, u(P_i) \tag{20}$$

where $\mathrm{d}K_0(z)/\mathrm{d}z = -K_1(z)$ and its limiting value $-1/z$ are applied. Equation (20) gives

$$a(P_i) = \theta(P_i)/(2\pi) \tag{21}$$

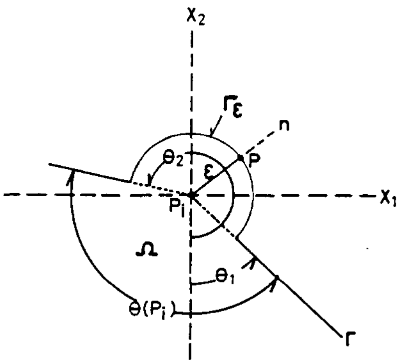

Fig. 1. Limiting process.

where $\theta(P_i)$ is the solid angle of Ω at the point P_i. In a similar way the three-dimensional case ($n = 3$) can be analyzed by use of (19).

5. Boundary element discretization

Suppose that the boundary Γ $(=\Gamma^{(1)} + \Gamma^{(2)})$ is divided into N boundary elements Γ_j ($j = 1, 2, \ldots, N$). In the constant discretization the nodal point P_j is taken at the center of Γ_j. In the linear discretization for $n = 2$ the nodal points P_j and P_{j+1} are taken at the edges of Γ_j where $P_1 = P_{N+1}$. In other words we have approximated $U(P)$ and $q(P)$ as

$$u(P) = \sum_{j=1}^{N} u(P_j) f_j(P) \tag{22a}$$

and

$$q(P) = \sum_{j=1}^{N} q(P_j) f_j(P) \tag{22b}$$

for $P \in \Gamma$, respectively, where $f_j(P)$ is the unit step function or linear shape function associated with P_j[1,2].

For simplicity we shall consider the case that the inhomogeneous term (or transformed heat source) (9) does not appear. The substitution of (22) into (13) then yields a system of linear equations in the form

$$[H]\{u(P_j)\} = [G]\{q(P_j)\} \tag{23}$$

where the $(i,\ j)$th components of $[H]$ and $[G]$ are respectively given by

$$H_{ij} = a(P_i)\delta_{ij} + \int_{\Gamma_j} q^*(P_i,\ P) f_j(P)\,\mathrm{d}\Gamma \tag{24a}$$

and

$$G_{ij} = \int_{\Gamma_j} w^*(P_i,\ P) f_j(P)\,\mathrm{d}\Gamma \tag{24b}$$

in which δ_{ij} $(i, j = 1, 2, \ldots, N)$ denotes the Kronecker's delta. For the calculation of these components (24a) and (24b) the Gaussian quadrature rule [1,2] are employed suitably. If we apply a uniform potential, e.g, $\{u(P_j)\} = \{1\}$ on the whole boundary Γ, we readily know $\{q\} = [G]^{-1}[H]\{1\} = \{0\}$. Thus $[H]$ becomes singular, while $[G]$ is nonsingular. In addition from the property of w^* and the form of (24b) $[G]$ is seen to be diagonally dominant. In general, both $[H]$ and $[G]$ are the $N \times N$ unsymmetric and full matrices. In the case that the inhomogeneous term (9) is included, we must introduce the internal cells [1,2] to Ω as well as the boundary elements. The resulting domain integrals in which the unknowns are not included (unlike [8,18]) can be evaluated by the Hammer's integration formula [2] efficiently. Note that the matrices $[H]$ and $[G]$ remain unchanged.

If the pure Dirichlet condition (10a) is only imposed on the whole boundary $\Gamma(=\Gamma^{(1)})$ in which $\Gamma^{(2)}$ is empty, then we can directly solve (23) without any rearrangement of $[H]$ and $[G]$. According to the splitting of Γ into $\Gamma^{(1)}$ and $\Gamma^{(2)}$, we rewrite (23) as

$$\begin{bmatrix} H^{(1,1)} & H^{(1,2)} \\ H^{(2,1)} & H^{(2,2)} \end{bmatrix} \begin{Bmatrix} u^{(1)} \\ u^{(2)} \end{Bmatrix} = \begin{bmatrix} G^{(1,1)} & G^{(1,2)} \\ G^{(2,1)} & G^{(2,2)} \end{bmatrix} \begin{Bmatrix} q^{(1)} \\ q^{(2)} \end{Bmatrix} \tag{25}$$

where the superscripts (1) and (2) denote the boundaries $\Gamma^{(1)}$ and $\Gamma^{(2)}$, respectively. The boundary conditions (10a) and (10b) are also discretized into

$$\{u^{(1)}\} = \{\bar{u}\} \quad \text{on} \quad \Gamma^{(1)} \tag{26a}$$

$$\{q^{(2)}\} = \{\bar{h}\} - \{V_n^{(2)} u^{(2)}\} \quad \text{on} \quad \Gamma^{(2)} \tag{26b}$$

by (22a) and (22b) where both $\{u^{(2)}\}$ and $\{q^{(2)}\}$ are the unknowns on $\Gamma^{(2)}$. Substituting (26a) and (26b) into (25) and rearranging (25), we obtain

$$\begin{bmatrix} -G^{(1,1)} & H^{(1,2)} + V_n^{(2)} G^{(1,2)} \\ -G^{(2,1)} & H^{(2,2)} + V_n^{(2)} G^{(2,2)} \end{bmatrix} \begin{Bmatrix} q^{(1)} \\ u^{(2)} \end{Bmatrix} = \begin{bmatrix} -H^{(1,1)} & G^{(1,2)} \\ -H^{(2,1)} & G^{(2,2)} \end{bmatrix} \begin{Bmatrix} \bar{u} \\ \bar{h} \end{Bmatrix} \tag{27}$$

in which the right-hand side is the known boundary data.

Therefore (27) can be written into the form

$$[A]\{X\} = \{B\} \tag{28}$$

where $[A]$ is the $N \times N$ given matrix, $\{X\}$ is the $N \times 1$ vector $\{q^{(1)} u^{(2)}\}^{t}$ to be determined and $\{B\}$ is the $N \times 1$ given vector. Once (28) has been solved by the elimination technique, $\{q^{(2)}\}$ is calculated from (26b). Thus we obtain all the boundary data $\{u(P_j)\}$ and $\{q(P_j)\}$. The internal solution $u(P_i)$ $(P_i \in \Omega)$ can be readily calculated from (13) with the weight $a(P_i) = 1$. Finally by use of the transformation formula (6) the original solution $\Phi(P_i)$ can be formed from the internal solution $u(P_i)$.

6. Numerical example

As an example in the numerical experiments we consider (3) over the unit square $\Omega = (0, 1) \times (0, 1)$ in which $V = (V_1, 0)$ is the x_1-directed constant vector. In addition the pure Dirichlet conditions

$$\begin{cases} \Phi(0, x_2) = \sin(\pi x_2), \\ \Phi(1, x_2) = \Phi(x_1, 0) = \Phi(x_1, 1) = 0, \end{cases} \tag{29}$$

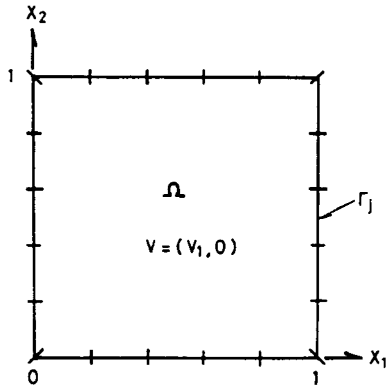

Fig. 2. Boundary element model $N = 20(= 5 \times 4)$.

are imposed on the whole boundary Γ. The Peclet number Pe is simply defined by

$$\mathrm{Pe} = 2V_1 \quad (>0) \tag{30}$$

which characterizes the numerical and exact solutions and designates the thickness (δ) of the boundary layer [14] in the x_1 direction as $\delta = 1/\sqrt{\mathrm{Pe}}$.

Figure 2. illustrates the boundary element model where Γ is regularly divided into N constant boundary elements. Figure 3 shows the boundary element solution along the straight line $x_2 = \frac{1}{2}$ where the Peclet number Pe = 80 and the thickness $\delta = 0.11180$. Here Ω is regularly divided into 100 bilinear finite elements for the standard and upwind finite element analyses. The present boundary element solution and the upwind finite element solution are stable, while the standard finite element solution is oscillatory in the whole domain Ω and especially in the boundary layer

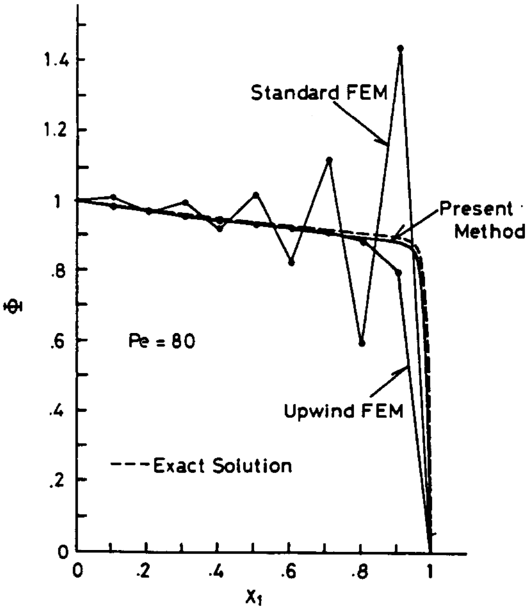

Fig. 3. Boundary element solution and other solutions.

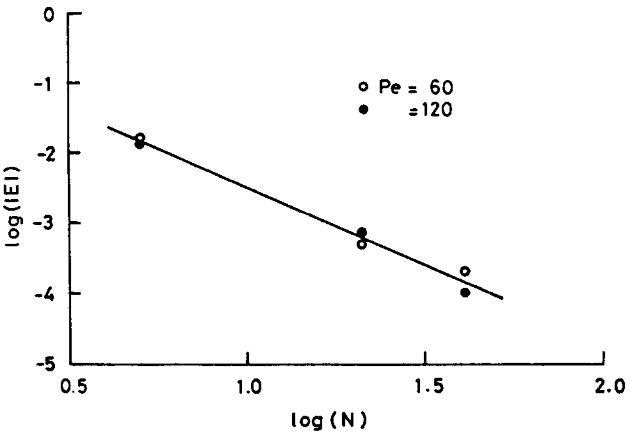

Fig. 4. Convergence characteristics of present boundary element method.

with the thickness δ. By a refinement of the finite elements in the boundary layer the standard finite element solution becomes stable [3], but the computational storage and cost will be extremely increasing. Moreover, in practical applications we cannot know generally where the boundary layers appear. On the other hand the upwind finite element method is more useful than the standard finite element method [4,12], but, as shown in Fig. 3 it does not always give accurate solutions. Figure 4 shows the convergence characteristics of the present method where E is the relative error at the center point $x_1 = x_2 = \frac{1}{2}$ in Ω. It is found out that the calculated boundary element solution is nearly with the second-order accuracy, and that its accuracy is independent upon the Peclet number Pe.

7. Concluding remarks

The boundary element method was presented for solving the steady convective diffusion equation in n dimension. For the formulation the governing operator was transformed into the selfadjoint or symmetric operator L under an assumption (7) on the flow potential Φ. In the present method this assumption is an essential part, but it will be valid in many practical applications. A simple example for the fundamental solution w^* is also given under the other assumption (14) on Φ, which is available to the analyses of the motional electromagnetic field as well as the uniform-flow fluid. The numerical result for a two-dimensional model problem ($n = 2$) was shown in order to demonstrate the usefulness of the present boundary element method. The boundary element solution was stable with respect to the large Peclet number Pe, and in particular it was more accurate in the boundary layer than the upwind finite element solution. In addition it was found out that the calculated internal solution for the constant boundary elements was with the second-order accuracy.

Therefore the present boundary element method will be useful and effective for a class of the steady convective diffusion problems. For more general potential flows a coupled boundary element method with the iterative method [15,16] may be effective, but it will always require the evaluation of domain integrals. The authors think that much efforts are needed to complete the boundary element method for the steady and transient convective diffusion problems.

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